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Supplementary Material

Cyano-functionalized diarylethene derivatives with aggregation induced emission enhancement and piezofluorochromic behaviors

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Contents:

Experiment section

General conditions

All the reagents were obtained commercially and used without further purification. ^{1}H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer using DMSO-d_6 as solvent. High resolution mass spectra were measured on a Bruker Paltonicsmicro TOF-QII instrument. IR spectra were acquired on Nicolet 380 FT-IR spectrometer. Photoluminescence spectra were recorded on Hitachi F-2500 spectrophotometer and photoluminescence spectra of solid state were measured by Horiba Jobin Yvon Fluorolog-3 spectrophotometer. Powder wide angle X-ray diffraction (PWXD) measurements were performed on a Miniflex 600 Powder X-ray diffractometer of Rigaku, operating at 40V, 40A, $4°min^{-1}$. Thermal gravimetric analysis (TGA) was conducted on TGA 128 instrument and differential scanning calorimetry (DSC) experiments were carried out on Perkin-Elmerat instrument, both of them were measured at a heating rate of 10ºC/min in nitrogen atmosphere.

Supporting data

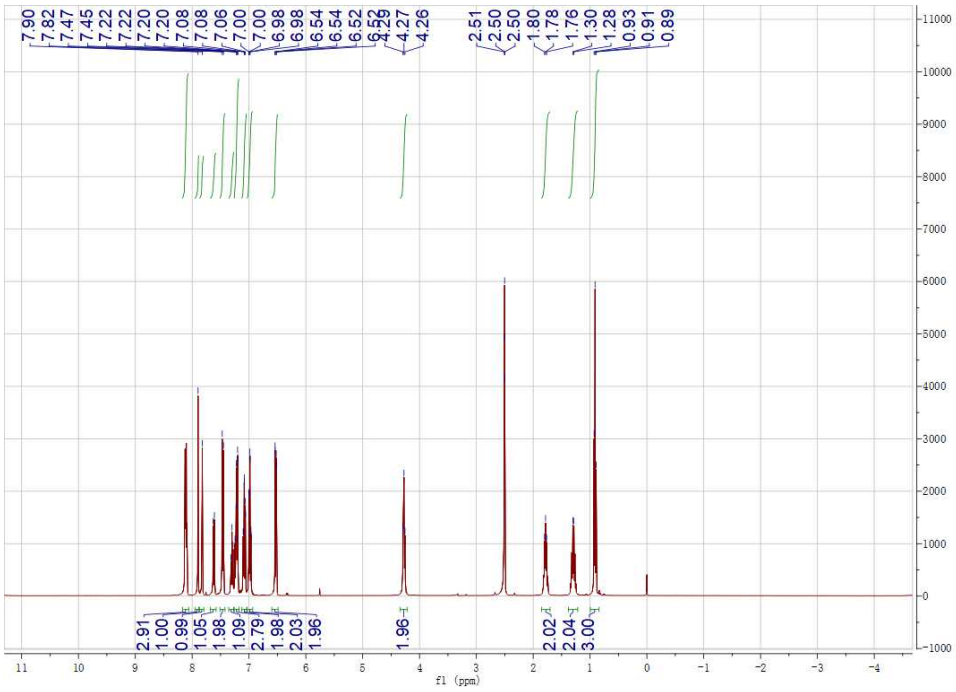

Fig. S1 (1) ^{1}H NMR spectra of PIA-4

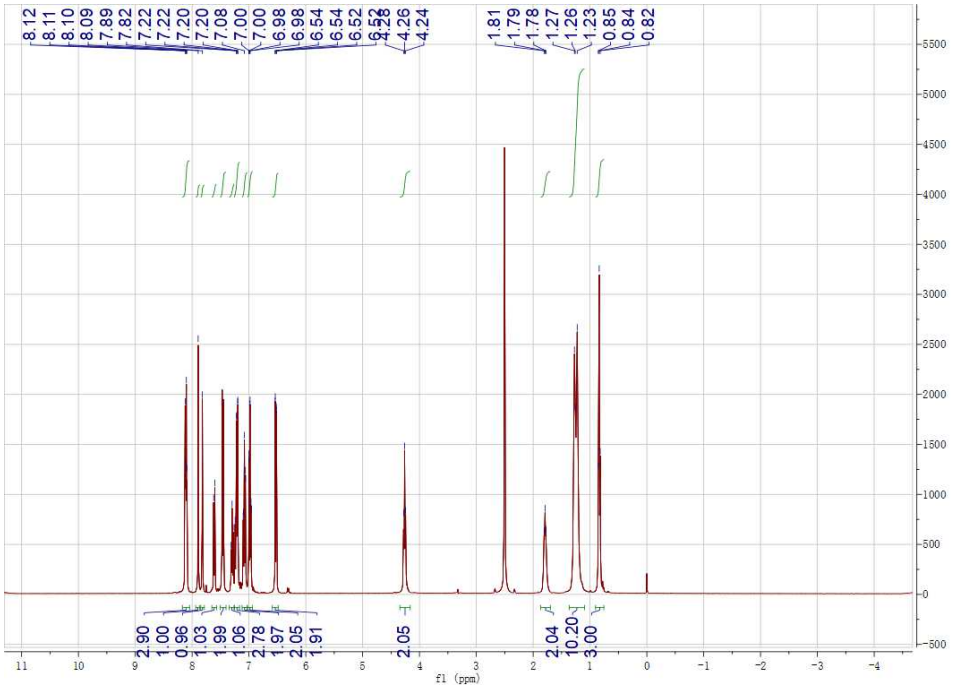

Fig. S1 (2) ^{1}H NMR spectra of PIA-8

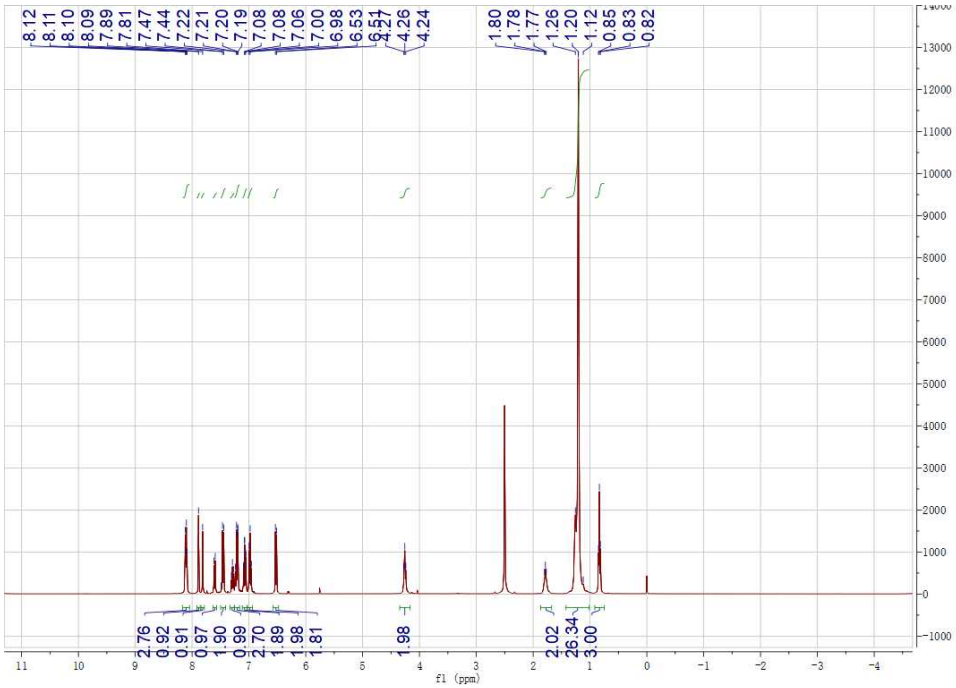

Fig. S1 (3) ^{1}H NMR spectra of PIA-12

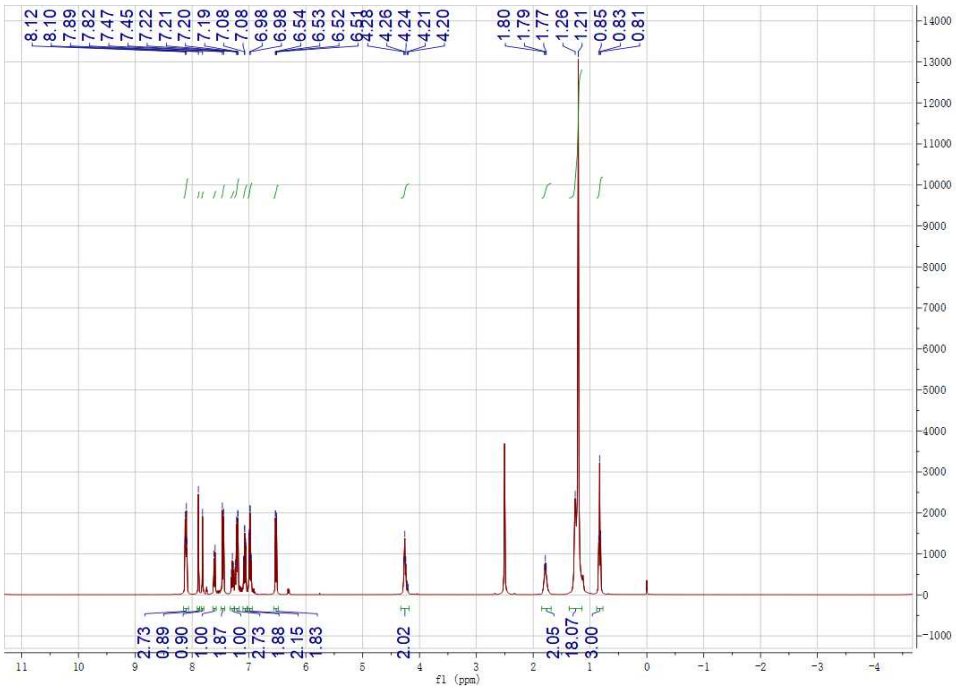

Fig. S1 (4) ^{1}H NMR spectra of PIA-16

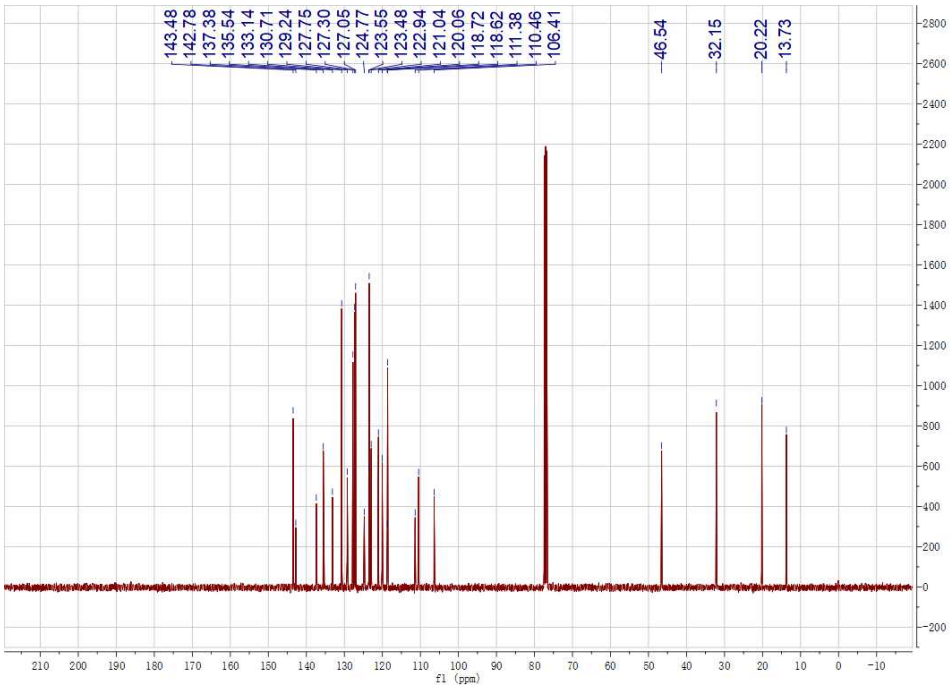

Fig. S2 (1) ^{13}C NMR spectra of PIA-4

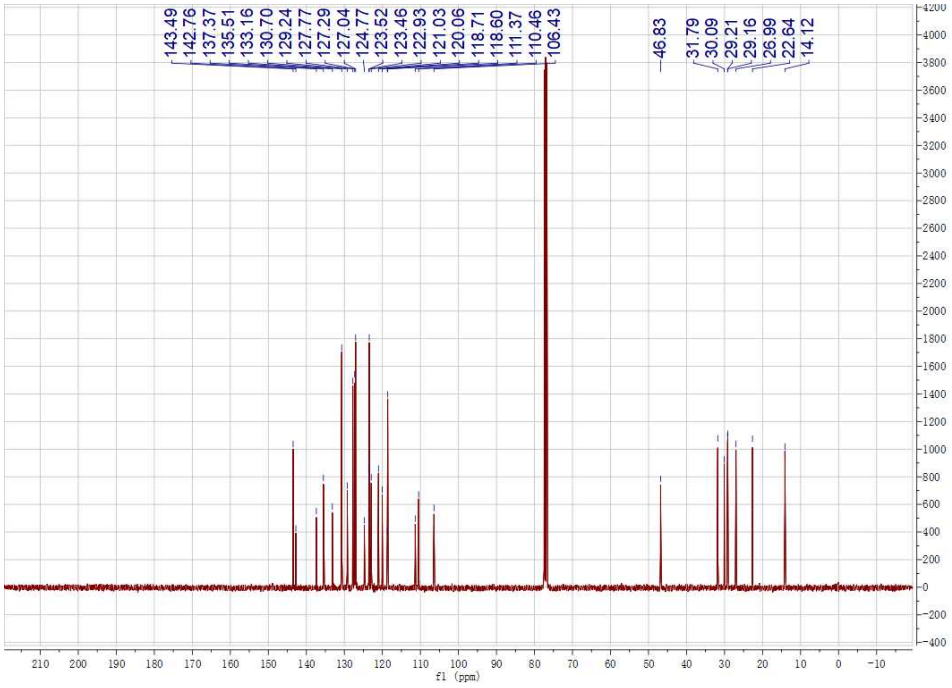

Fig. S2 (2) ^{13}C NMR spectra of PIA-8

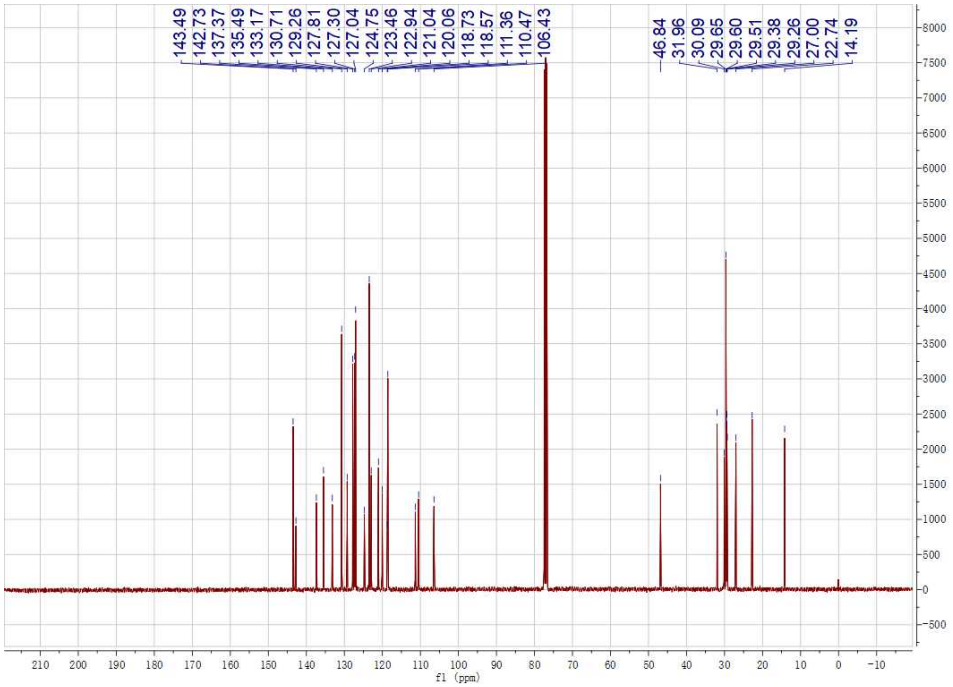

Fig. S2 (3) ^{13}C NMR spectra of PIA-12

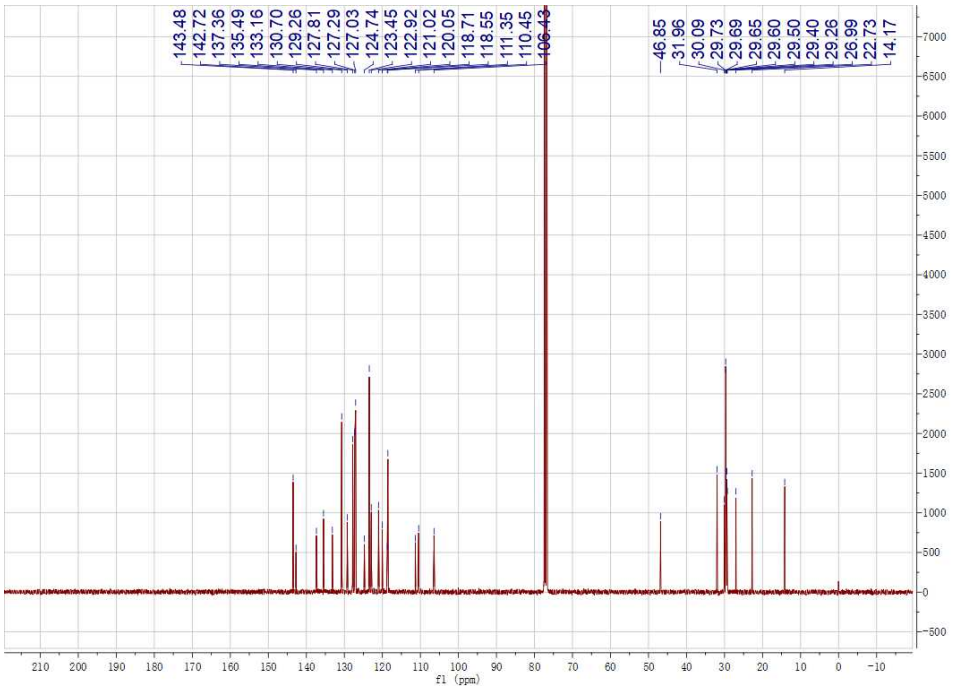

Fig. S2 (4) ^{13}C NMR spectra of PIA-16

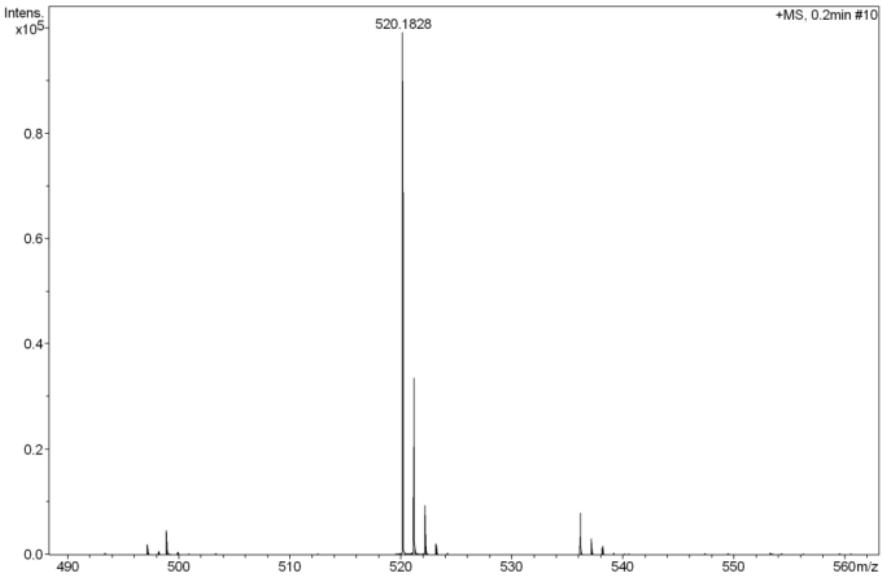

Fig. S3 (1) HRMS spectra of PIA-4

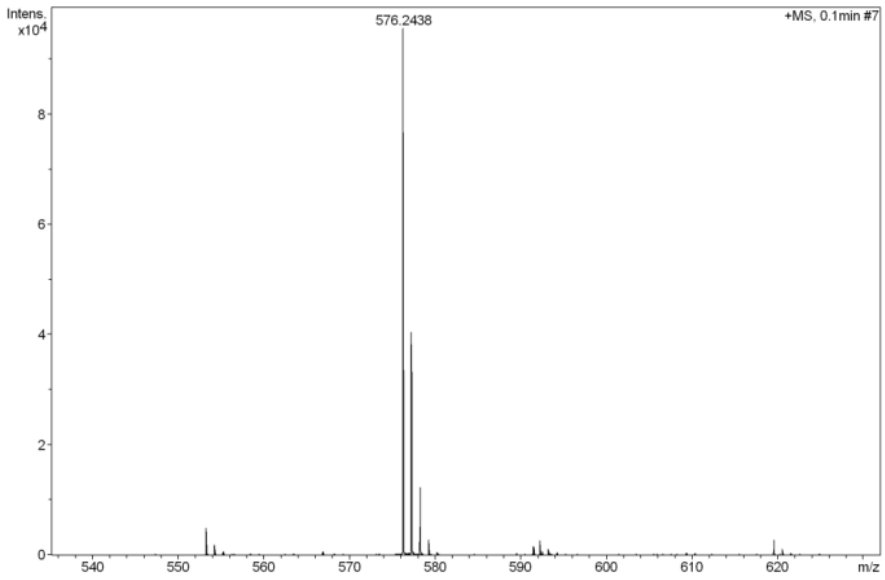

Fig. S3 (2) HRMS spectra of PIA-8

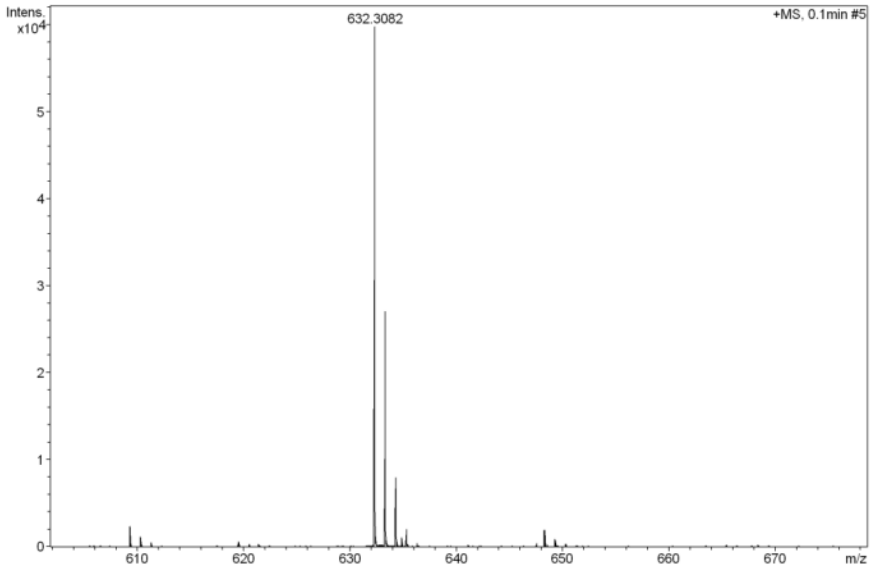

Fig. S3 (3) HRMS spectra of PIA-12

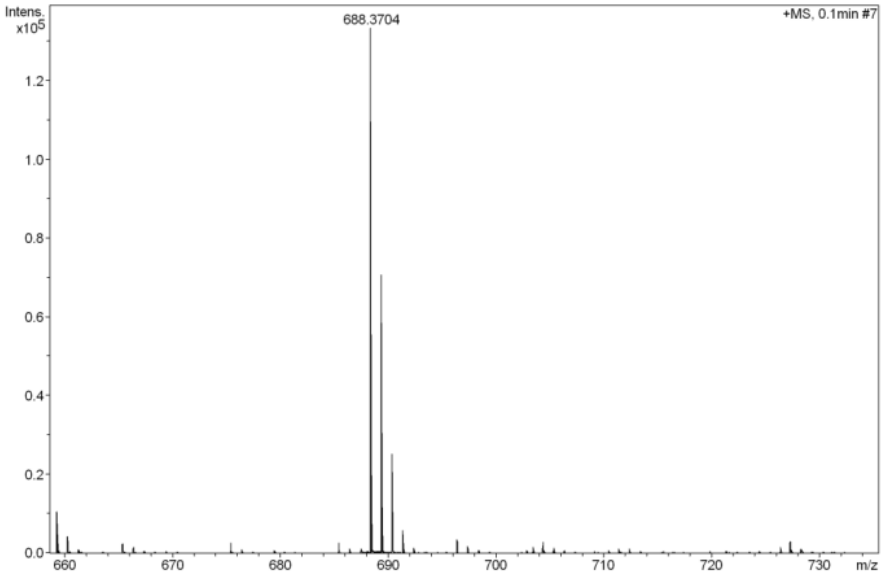

Fig. S3 (4) HRMS spectra of PIA-16

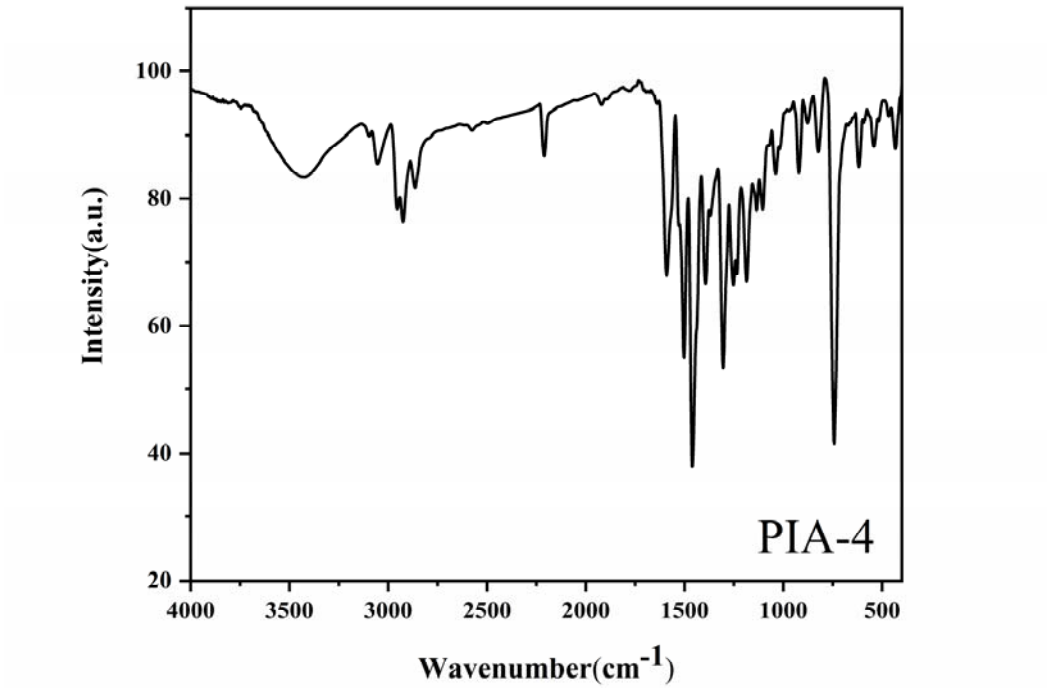

Fig. S4 (1) IR spectra of PIA-4

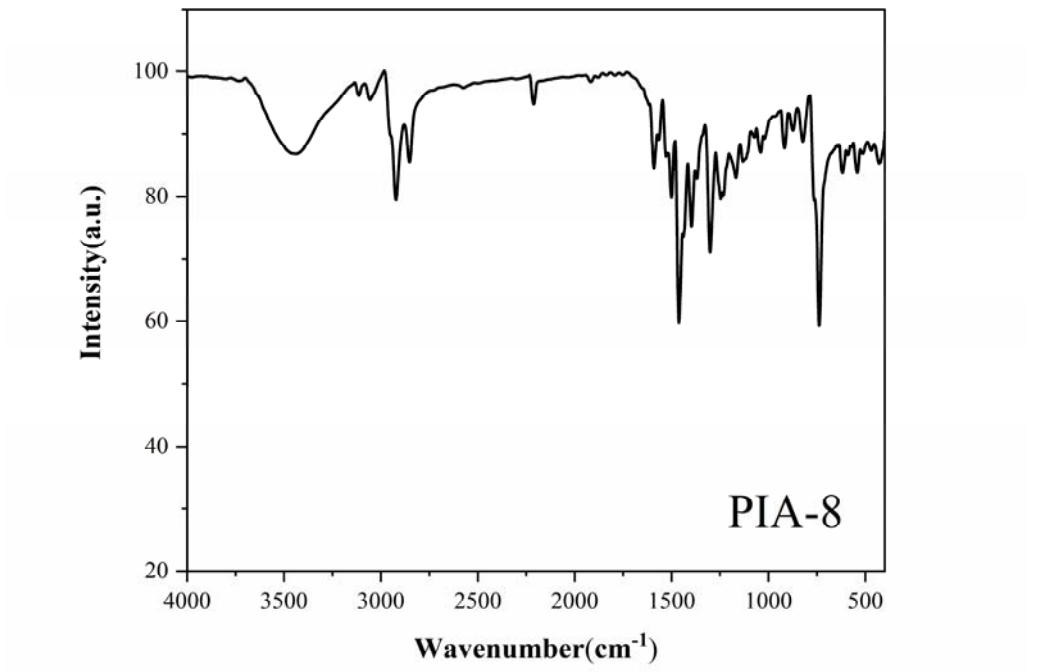

Fig. S4 (2) IR spectra of PIA-8

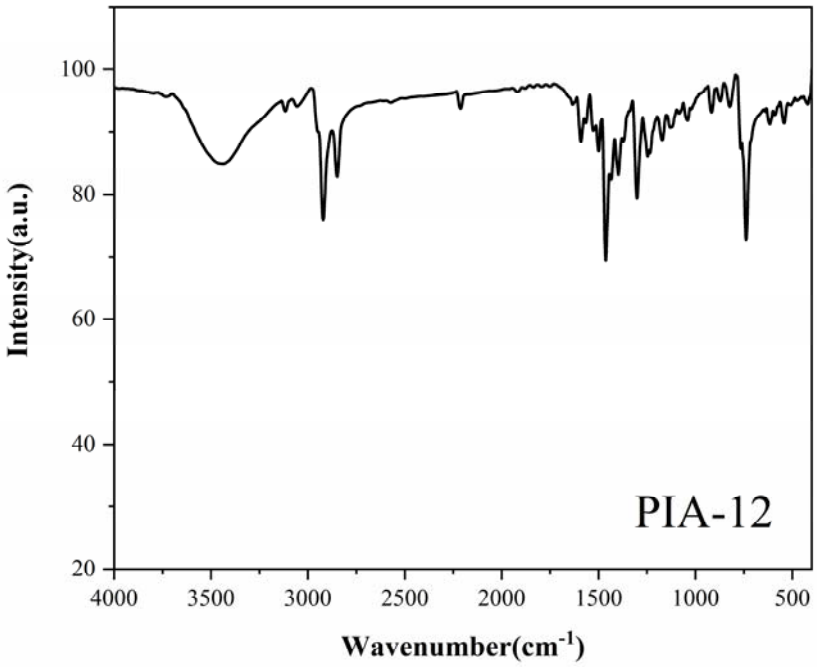

Fig. S4 (3) IR spectra of PIA-12

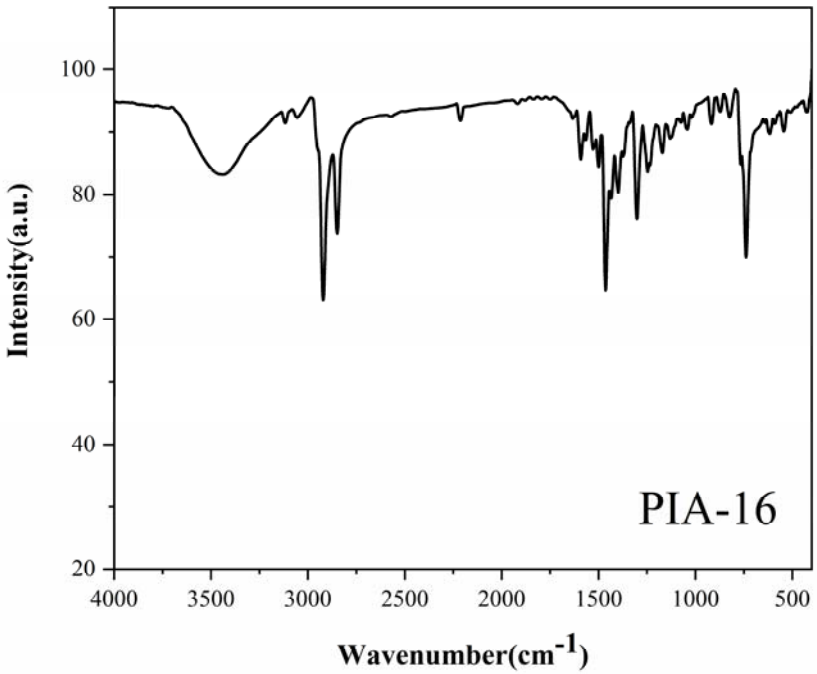

Fig S4 (4) IR spectra of PIA-16

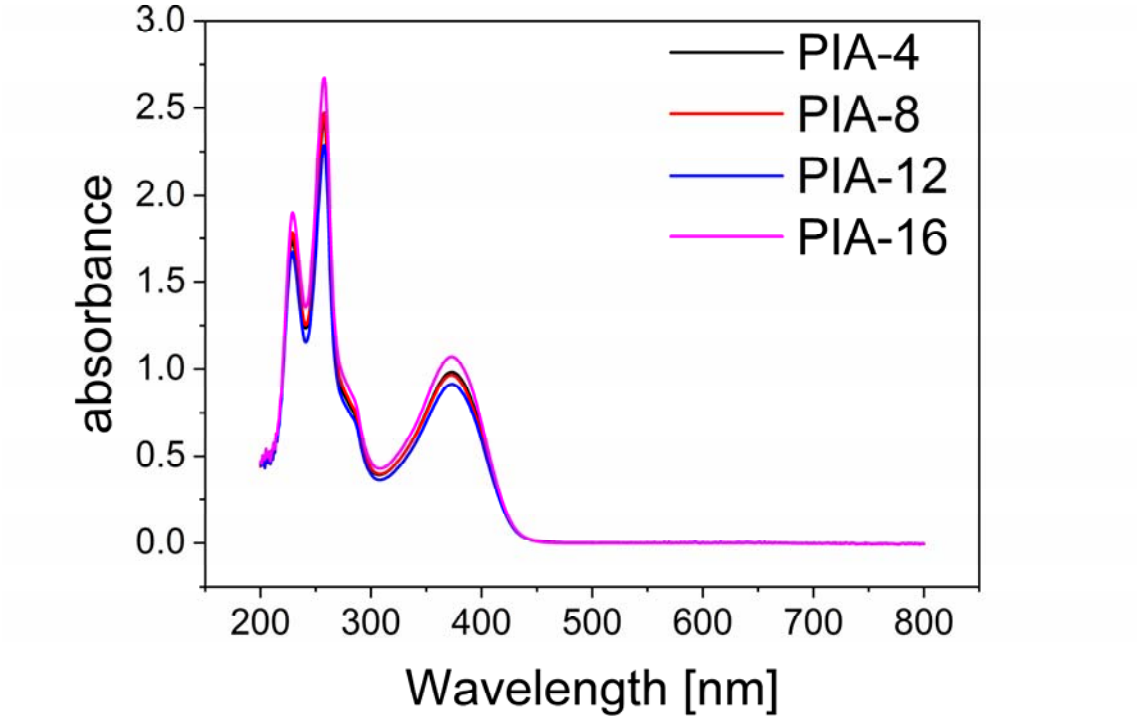

Fig. S5 UV absorption spectra of PIA-n in DCM.

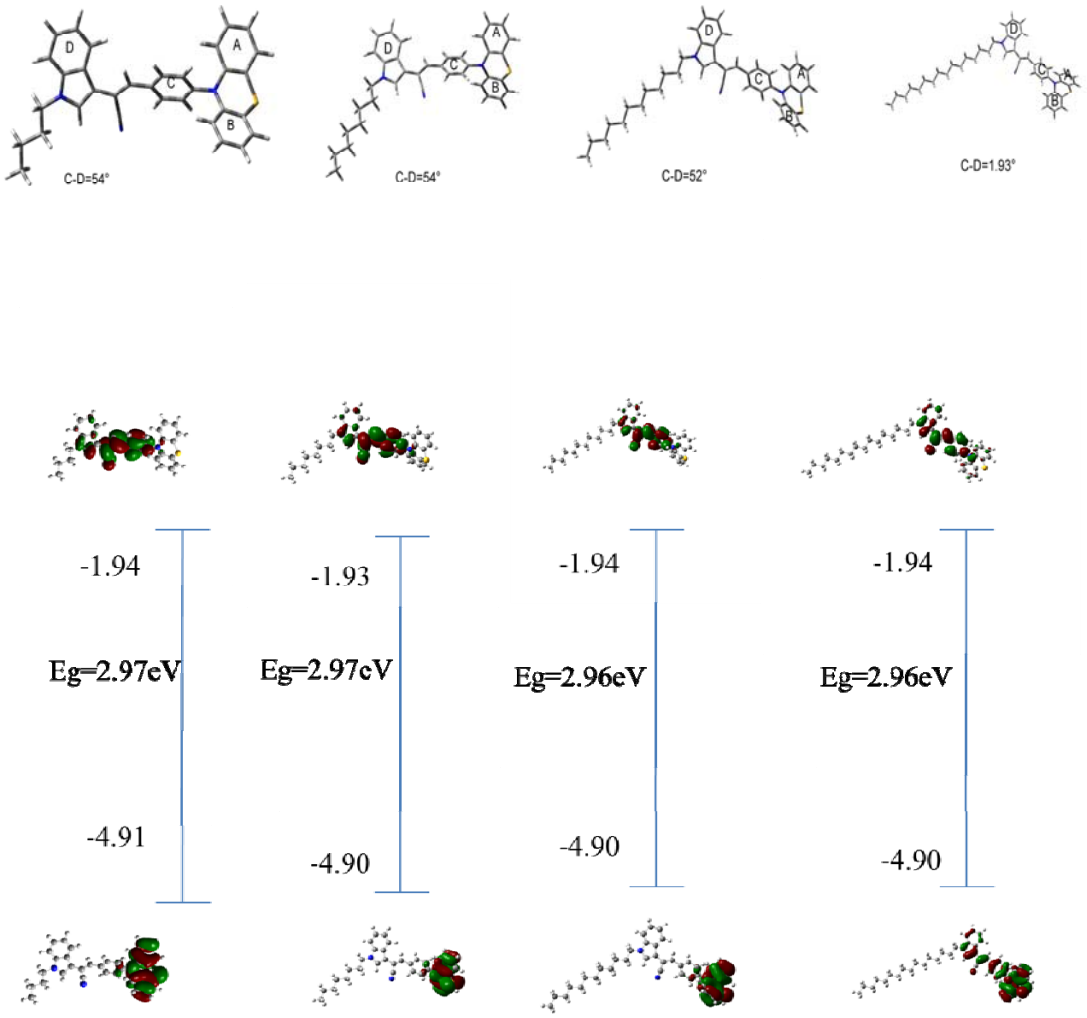

Fig. S6 Optimization geometry and calculated spatial electron distri-butions of HOMOs and LUMOs of PIA-4, PIA-8, PIA-12, PIA-16

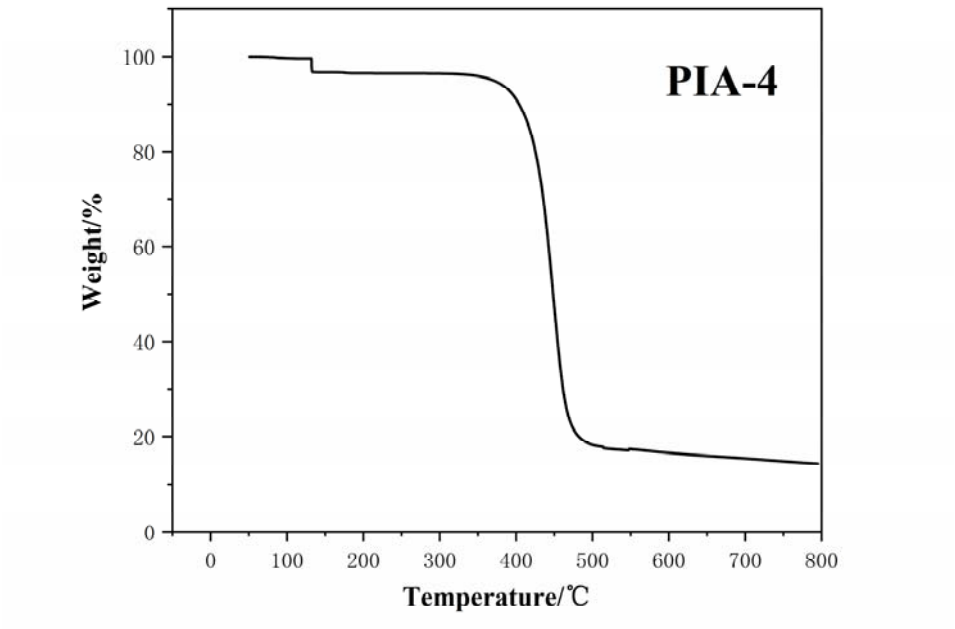

Fig. S7 (1) TGA curves of PIA-4

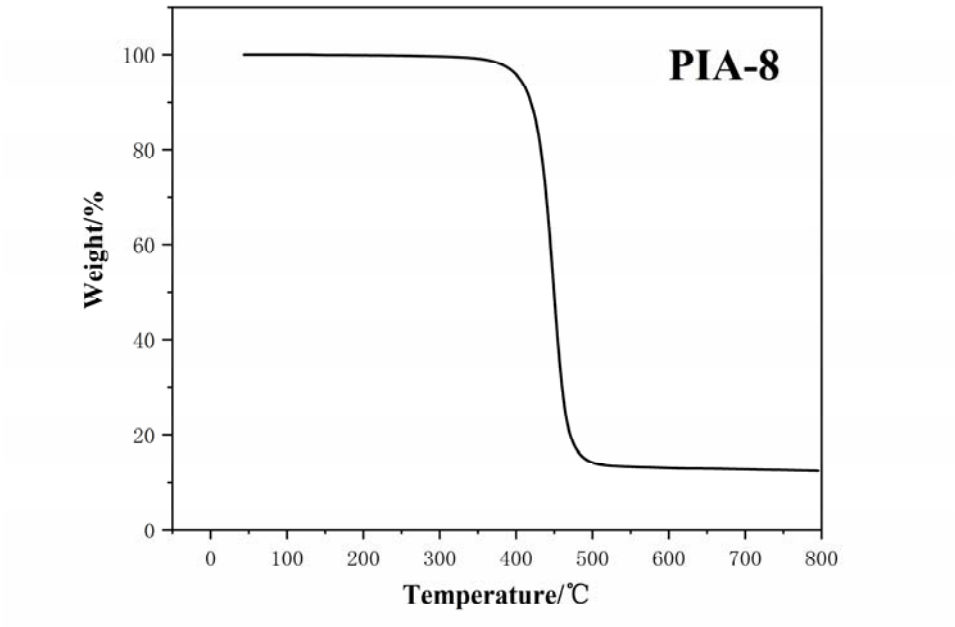

Fig. S7 (2) TGA curves of PIA-8

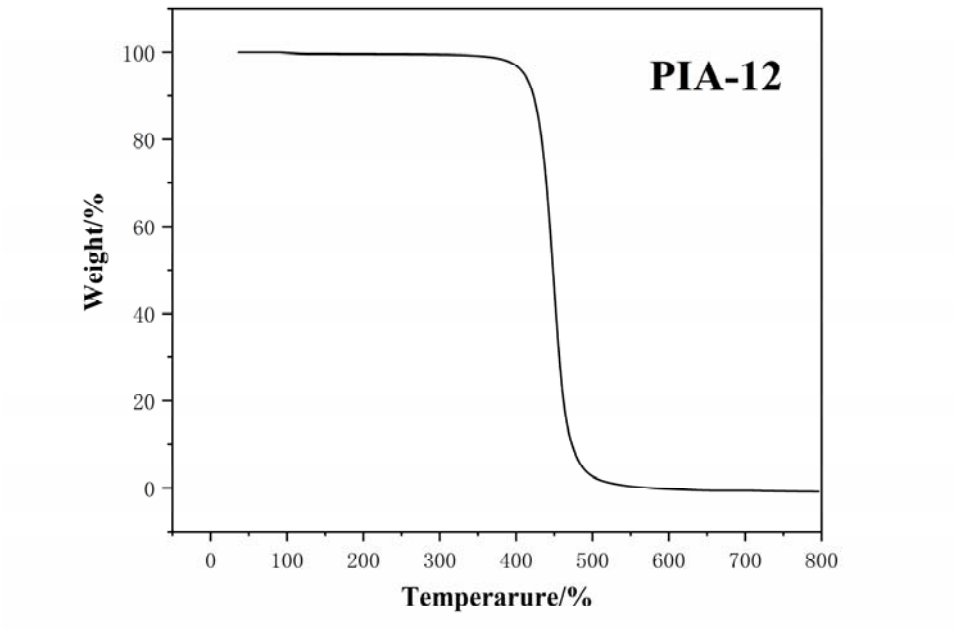

Fig. S7 (3) TGA curves of PIA-12

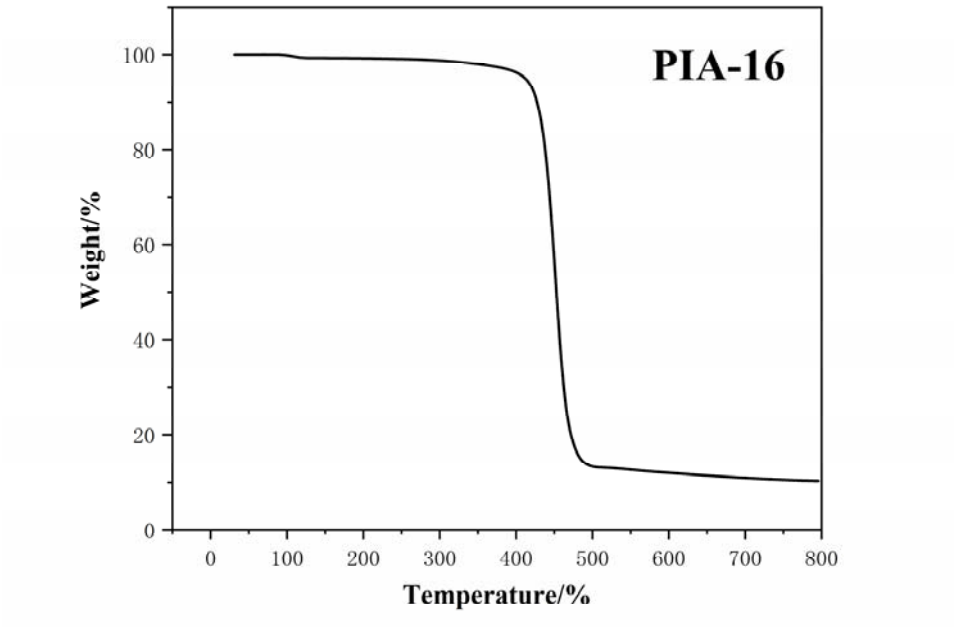

Fig. S7 (4) TGA curves of PIA-1

Table. S1 Crystal data and structure refinement for PIA-4.

Empirical formula	C_{33} H_{27} N_3 S
Formula weight	497.63
Temperature	113(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.131(3) A alpha = 90 deg.
	b = 19.775(4) A beta = 101.34(3) deg.
	c = 10.312(2) A gamma = 90 deg.
Volume	2625.3(10) A ^3
Z, Calculated density	4, 1.259 Mg/m^3
Absorption coefficient	0.150 mm^-1
F(000)	1048
Crystal size	0.200 x 0.180 x 0.120 mm
Theta range for data collection	1.887 to 27.837 deg.
Limiting indices	-17<=h<=17, -25<=k<=25, -13<=l<=13
Reflections collected / unique	31077 / 6230 [R(int) = 0.0666]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8778
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6230 / 0 / 336
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0644, wR2 = 0.1633
R indices (all data)	R1 = 0.0897, wR2 = 0.1828
Extinction coefficient	0.0095(17)
Largest diff. peak and hole	0.295 and -0.268 e.A^-3
CCDC	1857378